

eNanoMapper applications to support the risk assessment of nanomaterials

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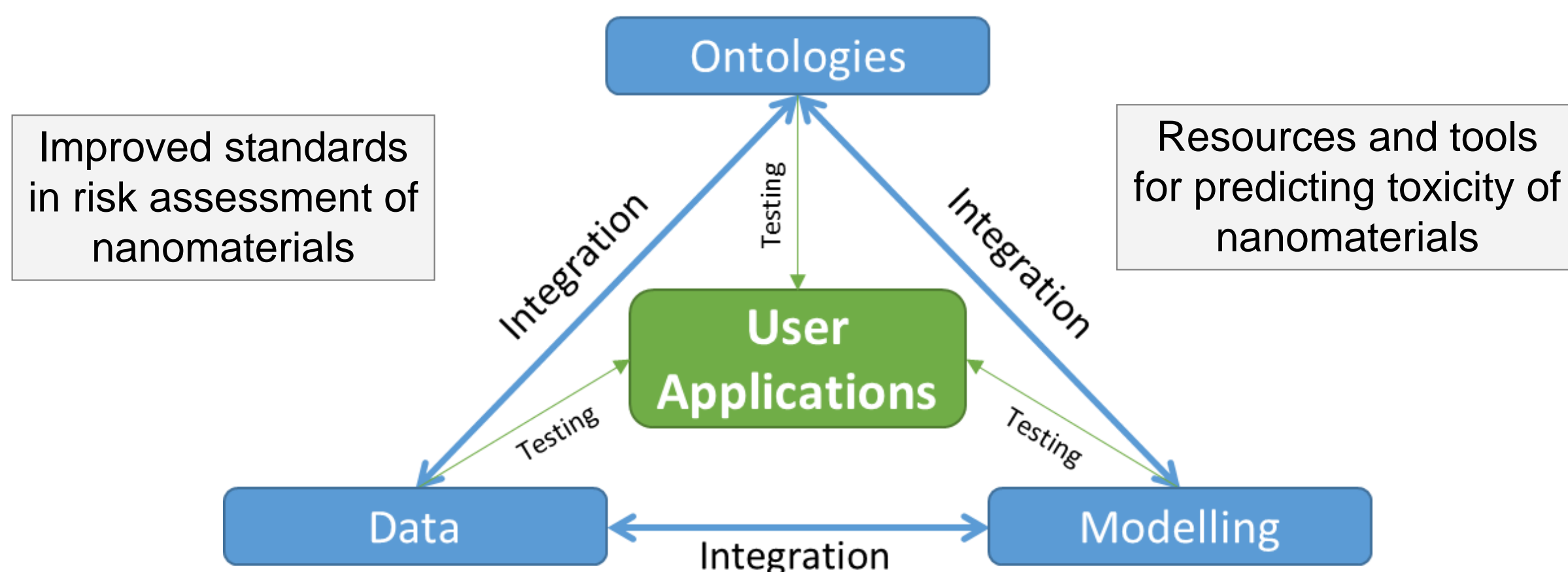


www.enanomapper.net



www.nanosafetycluster.eu

The infrastructure developed within eNanoMapper aims to support the data management in the area of nano safety research and to enable an **integrated approach for the risk assessment of nanomaterials**.



eNanoMapper developed an ontology, a data infrastructure and modelling tools with applicability in risk assessment of nanomaterials

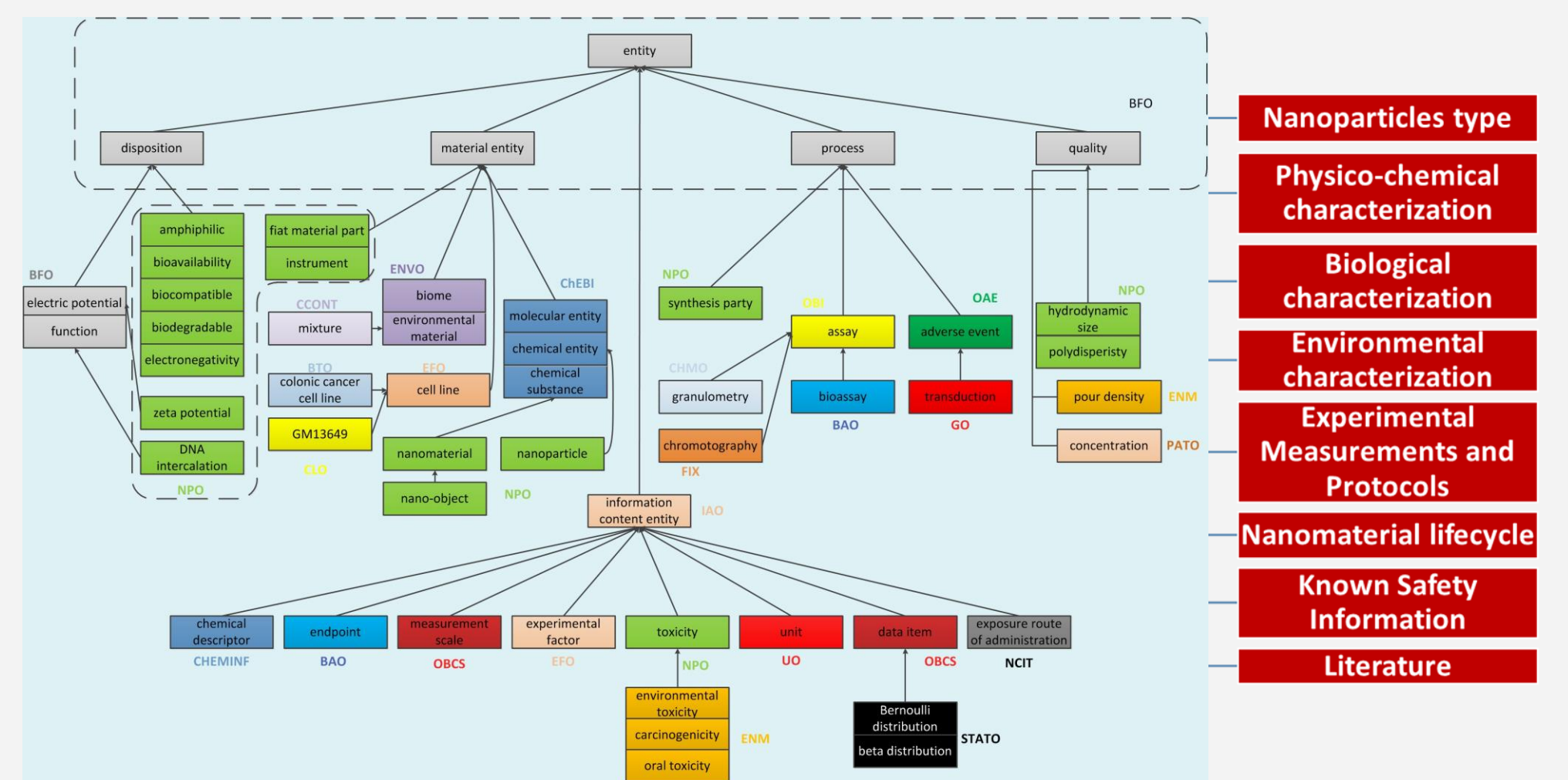
eNanoMapper provides a rich source of information and documentation (e.g. tutorials, webinars, publications) to support and guide the users.

<http://www.enanomapper.net/library>

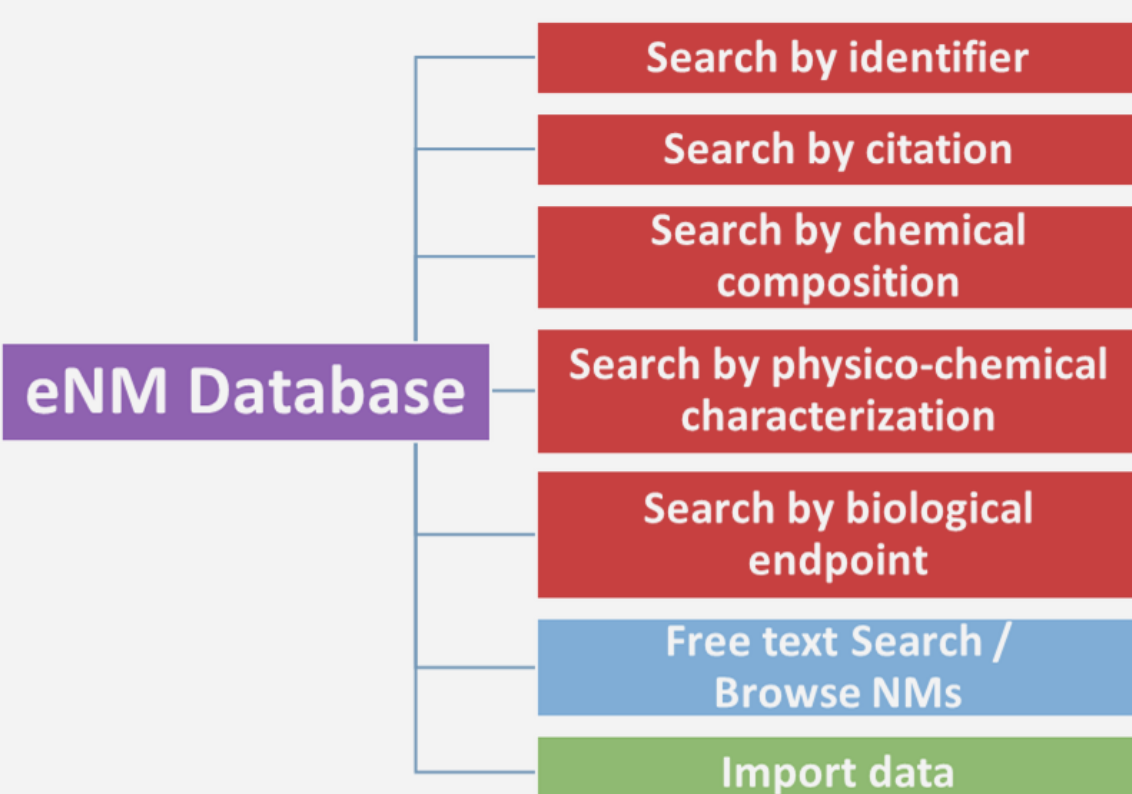
Ontologies

www.enanomapper.net/ontology

- The ontology includes common vocabulary terms used in nanosafety research and aims to provide a clear explanation of nanostructures based on information relating to their characterization, relevant experimental paradigms, biological interactions, safety indications and the integration of data from existing nanotoxicology sources.



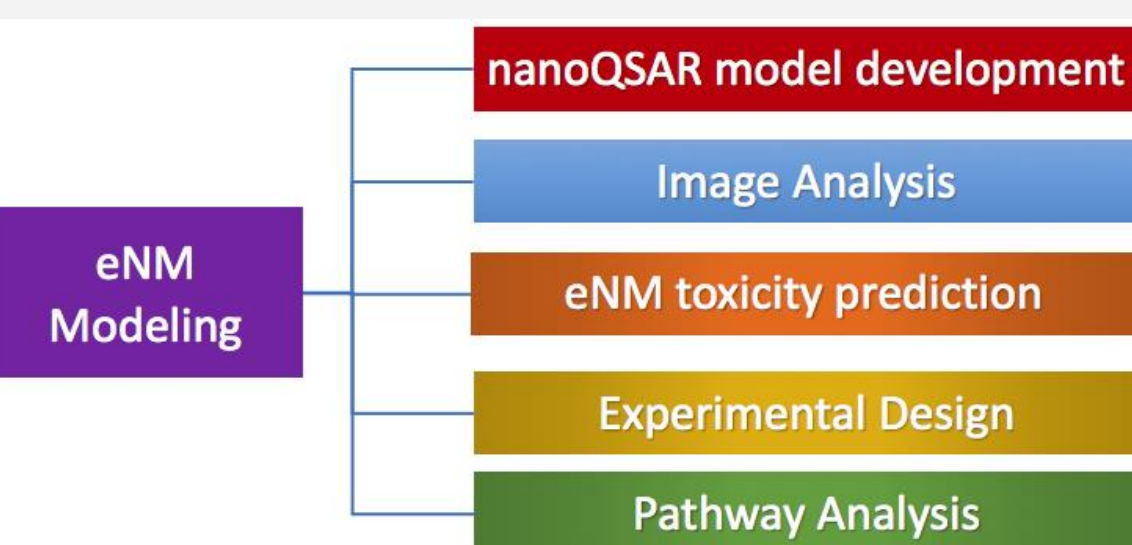
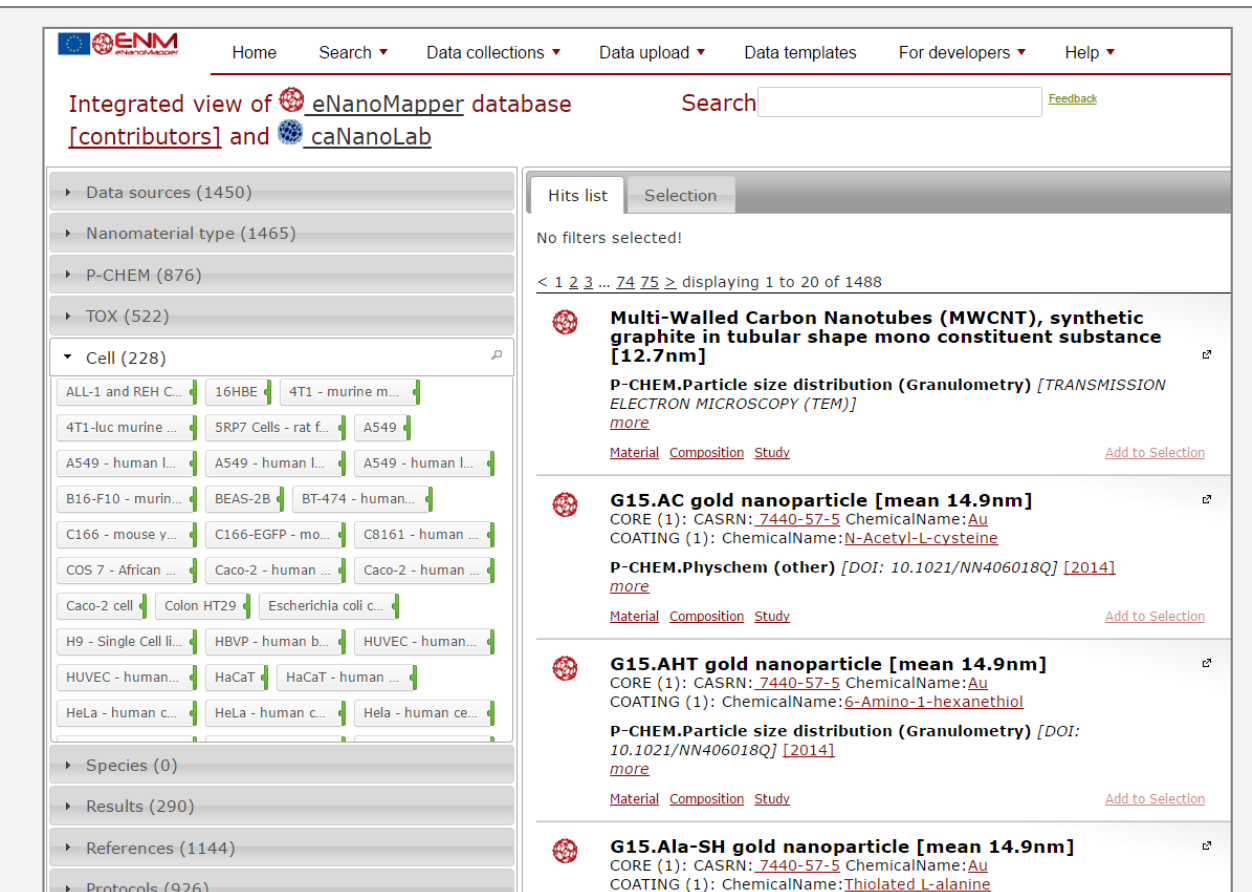
Overview of the upper levels and integration of external ontology content



Data

<https://data.enanomapper.net/>

- Public database demo hosting nanomaterials characterization data and biological and toxicological information.
- The database provides various possibilities to search and explore information, and to download data in various standard formats.
- Functionalities for data protection, data sharing, comparability and cross-talk with other databases.
- The database supports data upload in various formats, including configurable Excel templates.



Modelling

<http://www.enanomapper.net/modelling>

- Descriptors, computational toxicology models and modelling tools
- Enable the use and integration of nanosafety data from various sources.

JAQPOT QUATTRO

- The web application allows building QSAR models and using them for predictions. As an input, uses data available from eNanoMapper database. After preprocessing, transforming and preparing the datasets, the various modeling algorithms can be applied.

IMAGE DESCRIPTORS CALCULATION TOOL

- Tool for automated calculation of descriptors from images of nanomaterials. The tool provides the user with a systematic framework for the automated analysis of microscopy images of nanomaterials and the calculation of nanoparticle descriptors

RREGRS

- R package for computer-aided model selection for multiple regression methodologies by means of an extensive cross-validation scheme. It is used to find the best regression models for any numerical dataset.

TOXFLOW

- Web application for enrichment analysis and predictive read across modelling. If physicochemical and omics NP data are available both techniques can be applied in a sequential order

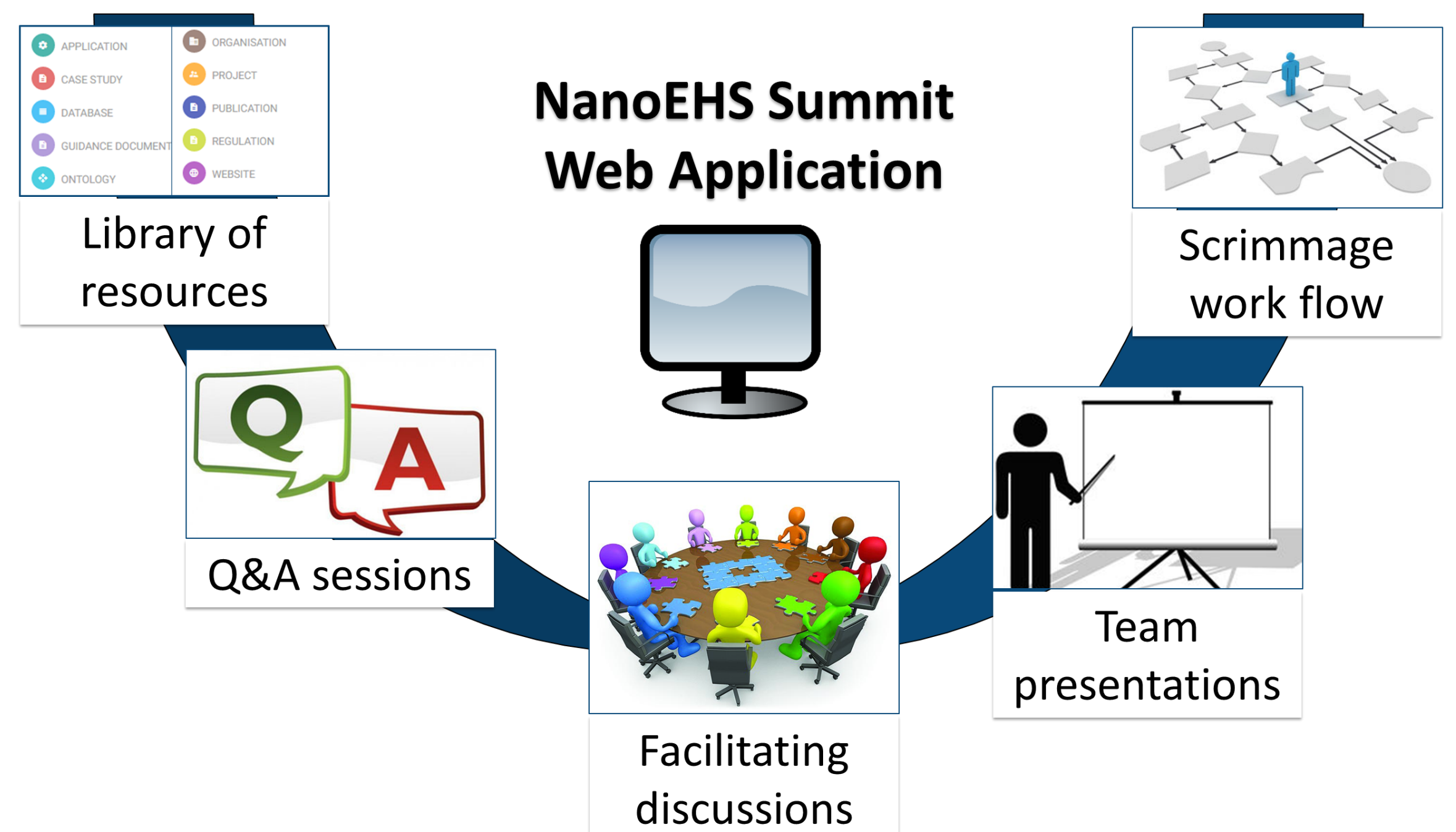
CHIPSTER FOR NANOMATERIAL-BASED OMICS DATA ANALYSIS

- An open source user-friendly analysis software for high-throughput data analysis. It offers over 350 bioinformatics tools and it is constantly updated according to the latest state-of-the-art tools and scripts.

NANO-LAZAR

- Modular framework for read across predictions of chemical toxicity

summit.eNanoMapper.net



Collaborative and support tool for nano-safety related events, with possible extension to other areas

Facilitates the interactions before, during and after the event:

- Add and create content and resources (e.g. publications, guidance documents)
- Add topics and questions to be discussed
- Add comments and answers related to the topics
- Gather information and capture the discussions
- Support the reporting

Hastings et al., eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment, Journal of Biomedical Semantics, March 2015, 10.1186/s13326-015-0005-5.

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Tsiliki et al., RRegrs: an R package for computer-aided model selection with multiple regression models. Journal of Cheminformatics 2015, 7:46.

Grafström et al., Toward the Replacement of Animal Experiments through the Bioinformatics-driven Analysis of 'Omics' Data from Human Cell Cultures. Altern Lab Anim. 2015 Nov;43(5):325-32.

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